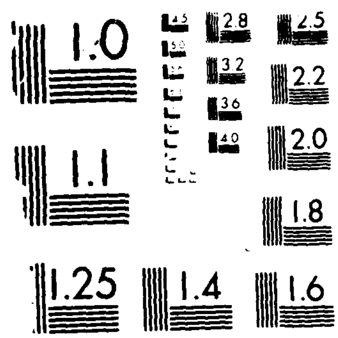
AD-A180 367 A MEASURE OF ROTATABILITY FOR RESPONSE SURFACE DESIGNS 1/1
(U) FLORIDA UNIV GAINESVILLE DEPT OF STATISTICS
A I KHURI MAY 87 TR-232 N00014-86-K-0059

UNCLASSIFIED F/G 12/4 NL



MICROCOPY RESOLUTION TEST CHART

A MEASURE OF ROTATABILITY FOR RESPONSE SURFACE DESIGNS

By

A. I. Khuri
Department of Statistics
University of Florida
Gainesville, FL 32611

Technical Report Number 232
May 1987

PREPARED UNDER GRANT NO. N00014-86-K-0059
FROM THE OFFICE OF NAVAL RESEARCH. ANDRE I. KHURI
AND RAMON C. LITTELL, PRINCIPAL INVESTIGATORS

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 232	2. GOVT ACCESSION NO. ADA180367	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) A Measure of Rotatability for Response Surface Designs		5. TYPE OF REPORT & PERIOD COVERED Technical Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) A. I. Khuri		8. CONTRACT OR GRANT NUMBER(s) N00014-86-K-0059 (R & T 4114552---01) Acct. No. 4910-1623459
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Statistics Nuclear Sciences Center University of Florida; Gainesville, FL 32611		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Mathematical Sciences Division (Code 411) Arlington, VA 22217-5000		12. REPORT DATE May 1987
		13. NUMBER OF PAGES 34
14. MONITORING AGENCY NAME & ADDRESS(If different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for Public Release: Distribution Unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Rotatable response surface designs; Percent rotatability; Repairing rotatability; Design moments; Cone of rotatability.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This paper introduces a measure which quantifies the amount of rotatability in a given response surface design. A technique is presented for increasing the value of this measure for nonrotatable designs.

A Measure of Rotatability for

Response Surface Designs

A. I. Khuri

Department of Statistics
University of Florida
Gainesville, FL 32611

ABSTRACT

A measure is introduced in this paper which quantifies the amount of rotatability in a given response surface design. The measure, which is expressible as a percentage, takes the value 100 if and only if the design is rotatable. One of the main advantages of this measure is that it can be used to "repair" a nonrotatable design by the addition of experimental runs which maximize the percent rotatability over a spherical region of interest. Four numerical examples are given to illustrate the applications of this measure.

KEY WORDS: Nonrotatable designs; Percent rotatability; Repairing rotatability; Design moments; Design augmentation; Cone of rotatability.

1. INTRODUCTION

Consider fitting a linear response surface model of order d in k input variables, $x_1, x_2, \ldots, x_k$, over a spherical region of interest, R, using a design consisting of n experimental runs. This model can be written in vector form as

$$E(\underset{\sim}{y}) = \underset{\sim}{X}\underset{\sim}{\beta}, \tag{1.1}$$

where $\underset{\sim}{y}$ is a vector of n observations, $E(\underset{\sim}{y})$ denotes the mean or expected value of $\underset{\sim}{y}$, $\underset{\sim}{X}$ is an $n \times p$ matrix of rank p whose elements are known functions of the design settings of the input variables, and $\underset{\sim}{\beta}$ is a vector of unknown regression coefficients. We assume that the variance-covariance matrix of $\underset{\sim}{y}$ is given by $\sigma^2 \underset{\sim}{I}_n$, where σ^2 is unknown and $\underset{\sim}{I}_n$ is the identity matrix of order $n \times n$. We denote by $\underset{\sim}{D}$ the $n \times k$ design matrix whose u^{th} row consists of the settings of the k input variables at the u^{th} experimental run $(u=1,2,\ldots,n)$.

The predicted response value at a particular point $\underset{\sim}{x} = (x_1, x_2, \ldots, x_k)'$ in the region R will be denoted by $\hat{y}(\underset{\sim}{x})$. This value is obtained by substituting the elements of $\underset{\sim}{\beta}$ in model (1.1) by the corresponding elements of $\hat{\underset{\sim}{\beta}}$, the least squares estimator of $\underset{\sim}{\beta}$, namely,

$$\hat{\underset{\sim}{\beta}} = (\underset{\sim}{X}'\underset{\sim}{X})^{-1}\underset{\sim}{X}'\underset{\sim}{y} \,. \tag{1.2}$$

The design $\underset{\sim}{D}$ is said to be rotatable if the variance of $\hat{y}(\underset{\sim}{x})$, which in general depends on $x_1, x_2, \ldots, x_k$, is a function of

only the distance of the point $\underset{\sim}{x}$ from the center of the design. Thus, when the design is rotatable, the prediction variance, denoted by $\mathrm{var}[\hat{y}(\underset{\sim}{x})]$, is the same at all points $\underset{\sim}{x}$ which are equidistant from the design center. Consequently, in the space of the input variables, surfaces of constant prediction variance form concentric hyperspheres (circles and spheres in two-dimensional and three-dimensional Euclidean spaces, respectively).

The concept of rotatability was first introduced by Box and Hunter (1957) and has since become an important design criterion. One of the desirable features of rotatability is that the quality of prediction, as measured by the size of $\mathrm{var}[\hat{y}(\underset{\sim}{x})]$, is invariant to any rotation of the coordinate axes in the space of the input variables. Furthermore, if optimization of $\hat{y}(\underset{\sim}{x})$ is desired over concentric hyperspheres within a certain region of interest, it would be very desirable to have a rotatable design. Otherwise, poor estimates of the optimum might result (see Khuri and Myers, 1979)

A simple characterization of rotatability is given in terms of the elements of the $\underset{\sim}{X}'\underset{\sim}{X}$ matrix. We shall refer to these elements as design moments (traditionally, the elements of the matrix $\underset{\sim}{X}'\underset{\sim}{X}/n$ are referred to as design moments). In general, a design moment for a model such as (1.1) of order d and in k input variables is denoted by $(1^{\delta_1} 2^{\delta_2} \ldots k^{\delta_k})$ and is equal to

$$(1^{\delta_1} 2^{\delta_2} \ldots k^{\delta_k}) = \sum_{u=1}^{n} x_{u1}^{\delta_1} x_{u2}^{\delta_2} \ldots x_{uk}^{\delta_k}, \tag{1.3}$$

where $\delta_1, \delta_2, \ldots, \delta_k$ are nonnegative integers and x_{uj} is the level of the j^{th} input variable used in the u^{th} experimental run ($j=1,2,\ldots,k$; $u=1,2,\ldots,n$). The sum, $\sum_{j=1}^{k} \delta_j$, is called the order of the design moment and is denoted by $\delta(\delta = 0,1,\ldots,2d)$. For example, $(1^2 3\ 5^3)$ is a design moment of order $\delta = 6$ and is equal to $\sum_{u=1}^{n} x_{u1}^2 x_{u3} x_{u5}^3$.

A necessary and sufficient condition for a design for fitting a model such as (1.1) (of order d and in k input variables) to be rotatable is that the design moments of order $\delta(\delta=0,1,\ldots,2d)$ be of the form

$$(1^{\delta_1} 2^{\delta_2} \ldots k^{\delta_k}) = \begin{cases} 0, & \text{if any } \delta_j \text{ is odd} \\ \dfrac{\theta_\delta \prod_{j=1}^{k} \delta_j!}{2^{\delta/2} \prod_{j=1}^{k} (\delta_j/2)!}, & \text{if all of the } \delta_j\text{'s are even,} \end{cases} \tag{1.4}$$

where θ_δ is a quantity which depends on d, δ, and n (see Box and Hunter 1957, Myers 1976, ch. 7). For convenience, we say that a design moment is odd if at least one of its δ_j's is odd and a design moment is even if all of the δ_j's are even. Note that a design moment of order $\delta = 0$ is equal to n. A design whose moments do not conform to formula (1.4) is said to be nonrotatable.

Quite often, a nonrotatable design may exhibit surfaces of constant prediction variance which are nearly spherical. In this case, the design is described s being near rotatable. This occurs, for example, when a rotatable design is deformed due to incorrect settings of some of the input variables, or because certain specified levels of the input variables may be difficult to employ in practice. In another situation, a rotatable design may undergo certain modifications to fit the needs of the experiment. The modifications might involve adding new design points, or shifting existing design points, in order to gain more information in a certain region of interest (see Littell and Mott 1974). In such situations it is of interest to assess the effects of deformation or modification on the property of rotatability.

To assess the degree of rotatability, it has been customary to inspect contour plots (in case of k=2 input variables) of constant prediction variance to see how close they are to being circular. Such a practice ,however, has its limitations when the number of input variables exceeds 3 in addition to being subjective. In this paper, we provide a quantitative measure of rotatability for a response surface design. This measure takes values between 0 and 100 with the latter value being attained when the design is rotatable. The proposed measure can be useful in the following situations:

(i) to quantify the degree of rotatability of a nonrotatable

design so that a determination of how "close" the design is to being rotatable can be made.

(ii) to compare designs on the basis of their degrees of rotatability.

(iii) to assess the extent of departure from rotatability when an already rotatable design is deformed or modified.

(iv) to repair a nonrotatable design.

2. A MEASURE OF ROTATABILITY

Consider again the model given in (1.1), which if we recall is of order d in the input variables $x_1, x_2, \ldots, x_k$. Let us suppose that in the spherical region R over which this model is fitted the input variables have been coded so that

$$\sum_{u=1}^{n} z_{uj} = 0, \qquad j=1,2,\ldots,k$$
$$\sum_{u=1}^{n} z_{uj}^2 = a, \qquad j=1,2,\ldots,k, \tag{2.1}$$

where z_{uj} denotes the coded value of x_{uj}, the actual value of the u^{th} level of variable j, and a is some positive constant. The coding can be accomplished by applying the transformation, $z_{uj} = (x_{uj} - \bar{x}_j)/s_j$, where $\bar{x}_j = \sum_{u=1}^{n} x_{uj}/n$ and s_j is given by $s_j = [\sum_{u=1}^{n} (x_{uj} - \bar{x}_j)^2/a]^{1/2}$.

By adapting the notation described in (1.3) to the coded variables,

the equalities described in (2.1) can be written as

$$(j) = 0 \quad , \qquad j = 1,2,\ldots,k,$$
$$(j^2) = a \quad , \qquad j = 1,2,\ldots,k. \tag{2.2}$$

Under this coding scheme, the center of the design coincides with the point at the origin of the coordinates system. The coding also helps to standardize the input variables which may have different units of measurements. Furthermore, the spread of the design will be the same in all directions of the coordinate axes.

In terms of the coded variables, model (1.1) can be expressed as

$$E(\underset{\sim}{y}) = \underset{\sim}{Z}\,\underset{\sim}{\gamma} \ , \tag{2.3}$$

where the matrix $\underset{\sim}{Z}$ is of the same form as $\underset{\sim}{X}$ except that the z_{uj}'s are used instead of the x_{uj}'s, and $\underset{\sim}{\gamma}$ is the new regression coefficient vector. Throughout the remainder of this paper, the design moments defined in (1.3) will be formulated in terms of the coded variables.

We shall now introduce a measure of rotatability for a given response surface design. Such a measure should be

(i) a function of the levels of the input variables used in the design,

(ii) invariant to the value of the scale parameter, a, in formula (2.1)

(iii) invariant to the addition of points at the center of the design (which coincides with the origin of the coordinates

system by the coding scheme).

The reason for condition (ii) is that there can be an infinite number of designs that are derivative of one another by changing the value of a. Since such designs are not different with respect to rotatability, their measures of rotatability should be the same. As for condition (iii), rotatability depends only on design moments of order $\delta > 1$ and these remain invariant to the addition of center points.

Three major steps are involved in the development of the proposed measure of rotatability. Details of these three steps are given below.

Step 1: The Reduction of All Design Moments to Scale-Free Quantities

Let us denote by $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$ the vector consisting of the elements of $\underset{\sim}{Z}'\underset{\sim}{Z}$ which are located above the diagonal as well as those along the diagonal. This vector is, therefore, of dimension $p^* = p(p+1)/2$, where p is the number of parameters in model (2.3). Its elements are obtained by listing the elements in the first row followed by those in the second row, etc., of the upper triangular half of $\underset{\sim}{Z}'\underset{\sim}{Z}$. It can be shown that the element at the $(i,j)^{th}$ location $(j \geq i)$ in this upper triangular half is the ℓ^{th} element of the vector $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$, where $\ell = f(i,j)$ is the function

$$f(i,j) = (i-1)[p-(i/2)] + j, \quad j > i. \tag{2.4}$$

For example, for a second-order model of the form

$$E(y) = \gamma_o + \gamma_1 z_1 + \gamma_2 z_2 + \gamma_{12} z_1 z_2 + \gamma_{11} z_1^2 + \gamma_{22} z_2^2,$$

$p = 6$, $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$ is of order 21×1, and the $(3,5)^{th}$ element of $\underset{\sim}{Z}'\underset{\sim}{Z}$, which is equal to the design moment $(1^2 2)$, is the 14^{th} element of $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$.

We note that the vector $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$ is scale dependent since it depends on the value of a used in formula (2.1). To remove this dependency, we divide each design moment of order $\delta(\delta = 0,1,\ldots,2d)$ by τ^{δ}, where τ is given by

$$\tau = \left[\sum_{j=1}^{k} (j^2)/k\right]^{1/2}, \tag{2.5}$$

that is, τ^2 is the average of all even design moments of order 2. We note that by the coding scheme described in (2.2), $\tau = a^{1/2}$. This operation amounts to premultiplying $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$ by a diagonal matrix, denoted by $\underset{\sim}{\Delta}$, of order $p^* \times p^*$. The diagonal elements of $\underset{\sim}{\Delta}$ are in a one-to-one correspondence with the elements of $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$: If an element of $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$ is a design moment of order $\delta(\delta=0,1,\ldots,2d)$, then the corresponding diagonal element of $\underset{\sim}{\Delta}$ is equal to $1/\tau^{\delta}$. Hence, the elements of the vector

$$\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z}) = \underset{\sim}{\Delta}\, \underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z}) \tag{2.6}$$

are scale-free quantities.

Step 2: The Introduction of a Canonical Representation of the $\underset{\sim}{Z}'\underset{\sim}{Z}$ Matrix for a Rotatable Design

If the design for model (2.3) is rotatable, then its design moments of order $\delta(\delta = 0,1,\ldots,2d)$ must have the special form described in (1.4). Hence, all the elements of $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$ corresponding to odd design moments should be equal to zero and all those corresponding to even design moments must have the form $\theta_\delta c(\delta_1,\delta_2,\ldots,\delta_k)$, where

$$c(\delta_1,\delta_2,\ldots,\delta_k) = \frac{\prod_{j=1}^{k} \delta_j!}{2^{\delta/2}\prod_{j=1}^{k}(\delta_j/2)!}, \quad \sum_{j=1}^{k}\delta_j = \delta(\delta=0,2,\ldots,2d). \qquad (2.7)$$

Let $\underset{\sim}{Z}_r$ denote the $\underset{\sim}{Z}$ matrix when the design is rotatable. In this case the vector $\underset{\sim}{v}(\underset{\sim}{Z}_r'\underset{\sim}{Z}_r)$ can be represented as

$$\underset{\sim}{v}(\underset{\sim}{Z}_r'\underset{\sim}{Z}_r) = \theta_0\underset{\sim}{\omega}_0 + \theta_2\underset{\sim}{\omega}_2 + \ldots + \theta_{2d}\underset{\sim}{\omega}_{2d}, \qquad (2.8)$$

where $\underset{\sim}{\omega}_\delta(\delta=0,2,\ldots,2d)$ is a vector of order $p^*\times 1$ whose elements are in a one-to-one correspondence with the elements of $\underset{\sim}{v}(\underset{\sim}{Z}_r'\underset{\sim}{Z}_r)$: All those corresponding to design moments of order different from δ and odd design moments of order δ are equal to zero, whereas those corresponding to even design moments of order δ have values given by formula (2.7). In other words, $\underset{\sim}{\omega}_\delta$ depends only on the values of the δ_j's which designate the even design moments of order $\delta(\delta=0,2,\ldots,2d)$ of a rotatable design. From (2.7) we note that the elements of $\underset{\sim}{\omega}_0$ are all zero except for the first element

which is equal to one. Also, from (1.4) it can be seen that $\theta_0 = n$ and that $\theta_2 = a$ by the coding scheme of formula (2.2). Hence, by (2.5), $\theta_2 = \tau^2$.

Since the elements of the diagonal matrix $\underset{\sim}{\Delta}$ in (2.6) that correspond to design moments of order δ are equal to $1/\tau^{\delta}$, then from (2.6) and (2.8) the following canonical representation of $\underset{\sim}{u}(\underset{\sim}{Z}_r'\underset{\sim}{Z}_r)$ can be obtained:

$$\begin{aligned}\underset{\sim}{u}(\underset{\sim}{Z}_r'\underset{\sim}{Z}_r) &= \sum_{m=0}^{d} \theta_{2m}\, \underset{\sim}{\omega}_{2m}/\tau^{2m} \\ &= n\, \underset{\sim}{\omega}_0 + \underset{\sim}{\omega}_2 + \sum_{m=2}^{d} \kappa_{2m}\, \underset{\sim}{\omega}_{2m},\end{aligned} \tag{2.9}$$

where $\kappa_{2m} = \theta_{2m}/\tau^{2m}$, or equivalently,

$$\kappa_{2m} = \theta_{2m}/\theta_2^m\ ,\ m = 2,3,\ldots,d. \tag{2.10}$$

Since θ_{2m} is a design moment of order $\delta = 2m$ as can be seen from (1.4) by taking m of the δ_j's equal to 2 and the remaining δ_j's equal to zero, the κ_{2m}'s in (2.10) are, therefore, scale free. The parameters $\kappa_4, \kappa_6, \ldots, \kappa_{2d}$ can be chosen by the experimenter depending on whatever additional properties the rotatable design is required to have. It is to be noted that the $\underset{\sim}{\omega}_{2m}$'s $(m=0,1,\ldots,d)$ in (2.9) are pairwise orthogonal, that is, $\underset{\sim}{\omega}_{2m}'\, \underset{\sim}{\omega}_{2m'} = 0$ for $m \neq m'$. This follows from the fact that all the elements of $\underset{\sim}{\omega}_{2m}$ are zero except for those corresponding to even design moments of order 2m. For these latter elements, the corresponding elements of $\underset{\sim}{\omega}_{2m'}$, for $m \neq m'$, must be zero by

definition. Consequently, the vectors $\underset{\sim}{\omega}_4, \underset{\sim}{\omega}_6, \ldots, \underset{\sim}{\omega}_{2d}$ span a (d-1)-dimensional Euclidean space. Furthermore, since $\kappa_{2m} > 0$ for m=2,3,...,d, then

$$\underset{\sim}{\nu} = \sum_{m=2}^{d} \kappa_{2m} \underset{\sim}{\omega}_{2m} \tag{2.11}$$

represents a vector in a closed convex cone K in this Euclidean space. By definition, a closed subset S of a Euclidean space is a closed convex cone if for any vectors, $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$, in S and any nonnegative scalars, λ_1 and λ_2, the vector $\lambda_1 \underset{\sim}{x}_1 + \lambda_2 \underset{\sim}{x}_2$ belongs to S. We shall refer to the cone K as the cone of rotatability.

Step 3: <u>The Derivation of the Rotatability Measure</u>

Let us now suppose that we have an n-point design, $\underset{\sim}{D}$, not necessarily rotatable, for fitting model (2.3). As before, the input variables are coded as in (2.2). The corresponding vector $\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z})$ in (2.6) can then be written as

$$\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z}) = n\,\underset{\sim}{\omega}_0 + \underset{\sim}{\omega}_2 + \underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z}), \tag{2.12}$$

where $\underset{\sim}{\omega}_0$ and $\underset{\sim}{\omega}_2$ are the same as in (2.9), which holds for a rotatable design having the same number, n, of runs. The elements of $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$ are equal to the corresponding elements of $\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z})$ except for those that correspond to design moments of order $\delta = 0$ and even design moments of order $\delta = 2$, which are equal to zero.

To measure the rotatability of the design $\underset{\sim}{D}$ it is necessary to determine how well the vector $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$ can be approximated with

a vector $\underset{\sim}{\nu}$ of the form given in (2.11). This is equivalent to finding a vector $\underset{\sim}{\nu} \in K$, the cone of rotatability described earlier, that is closest (in terms of the Euclidean norm) to $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$. For this purpose the parameters $\kappa_4, \kappa_6, \ldots, \kappa_{2d}$ in (2.11) are chosen so that

$$Q_n(\underset{\sim}{D}) = \| \underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z}) - \sum_{m=2}^{d} \kappa_{2m} \underset{\sim}{\omega}_{2m} \|^2 \qquad (2.13)$$

is minimum, where $\|\cdot\|$ denotes the Euclidean norm, or length, of a vector. In Appendix A it is shown that the minimum value of $Q_n(\underset{\sim}{D})$ is given by the formula

$$\min[Q_n(\underset{\sim}{D})] = \|\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2 - \sum_{m=2}^{d} [\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m}]^2/\|\underset{\sim}{\omega}_{2m}\|^2. \qquad (2.14)$$

It is interesting to note that with κ_{2m} being given as in (A.3) in Appendix A, the vector $\sum_{m=2}^{d} \kappa_{2m}\underset{\sim}{\omega}_{2m}$ is the projection of the vector $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$ on the cone of rotatability K. The square of the Euclidean norm of this projection is given by the absolute value of the second term on the right side of (2.14) and represents the portion of $\|\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2$ which can be attributed to rotatability. Hence, as a measure of rotatability for the design $\underset{\sim}{D}$ I choose the quantity

$$\begin{aligned}\Phi_n(\underset{\sim}{D}) &= 100\{\|\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2 - \min[Q_n(\underset{\sim}{D})]\}/\|\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2 \\ &= 100\{\sum_{m=2}^{d} [\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m}]^2/\|\underset{\sim}{\omega}_{2m}\|^2\}/\|\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2, \qquad (2.15)\end{aligned}$$

which represents the percent contribution of rotatability to the

magnitude of $\|\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2$. In other words, $\Phi_n(\underset{\sim}{D})$ represents the percent rotatability that is inherent in the design $\underset{\sim}{D}$. This is analogous to the use of the coefficient of determination, R^2, in regression, which measures the proportion of the total variation in the response that is caused by, or attributed to, the fitted model. If $\underset{\sim}{D}$ is rotatable, then $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$ must belong to the cone of rotatability K, hence $\min[Q_n(\underset{\sim}{D})] = 0$ and $\Phi_n(\underset{\sim}{D}) = 100$. A large value of $\Phi_n(\underset{\sim}{D})$ is, therefore, an indication that the design $\underset{\sim}{D}$ is near rotatable.

The measure of rotatability defined in (2.15) satisfies conditions (i), (ii), and (iii) stated earlier in this section. This follows from the fact that the vector $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$ is scale free and its elements depend on design moments of order two or higher, hence they are unaffected by the addition of center points.

3. REPAIRING ROTATABILITY

The measure developed in Section 2 can be used effectively to increase the percent rotatability of a nonrotatable design by augmenting it with additional runs chosen appropriately. This is particularly useful in situations where, because of technical limitations, some of the input variables of a rotatable design are set at levels different from those in the original design causing it to become nonrotatable. Also, it frequently happens that a rotatable design is purposely modified by the introduction of new

runs in order to concentrate information in certain areas of interest (see Littell and Mott 1974). This modification usually results in loss of rotatability.

The choice of points to be added to a nonrotatable design to increase its percent rotatability can be accomplished in a sequential manner as follows: Let $\underset{\sim}{D}^{(0)}$ denote a given nonrotatable design consisting of n_0 experimental runs. For any point, $\underset{\sim}{x}$, in the experimental region R, the design $\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}}$ consists of the design $\underset{\sim}{D}^{(0)}$ augmented with $\underset{\sim}{x}$. The percent rotatability of $\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}}$ is given by $\Phi_{n_0+1}(\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}})$. A new design point, $\underset{\sim}{x}_1$, is now added to $\underset{\sim}{D}^{(0)}$ to obtain the design $\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}_1}$. This new point is chosen by maximizing the percent rotatability of $\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}}$ with respect to $\underset{\sim}{x}$ over R. For simplicity the design $\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}_1}$ is written as $\underset{\sim}{D}^{(1)}$. We thus have

$$\Phi_{n_0+1}(\underset{\sim}{D}^{(1)}) = \max_{\underset{\sim}{x}\epsilon R}[\Phi_{n_0+1}(\underset{\sim}{D}^{(0)}_{\underset{\sim}{x}})].$$

A second design point, $\underset{\sim}{x}_2$, is subsequently added to $\underset{\sim}{D}^{(1)}$ by repeating the same process as above, but with $\underset{\sim}{D}^{(1)}$ replacing $\underset{\sim}{D}^{(0)}$. Let $\underset{\sim}{D}^{(2)}$ be the design consisting of $\underset{\sim}{D}^{(1)}$ augmented with $\underset{\sim}{x}_2$. By continuing this process we obtain the sequence of designs, $\underset{\sim}{D}^{(1)}, \underset{\sim}{D}^{(2)},\ldots,\underset{\sim}{D}^{(i)},\ldots$, where $\underset{\sim}{D}^{(i)}$ is obtained from $\underset{\sim}{D}^{(i-1)}$ by augmenting it with $\underset{\sim}{x}_i$ $(i=1,2,\ldots)$.

The percent rotatability associated with design $\underset{\sim}{D}^{(i)}$ is $\Phi_{n_i}(\underset{\sim}{D}^{(i)})$, where $n_i = n_0 + i$ $(i=0,1,\ldots)$. In Appendix B it is

shown that

$$\Phi_{n_i}(\underset{\sim}{D}^{(i)}) \leq \Phi_{n_{i+1}}(\underset{\sim}{D}^{(i+1)}), \quad i=0,1,\ldots \tag{3.1}$$

Inequality (3.1) implies that the sequence, $\{\Phi_{n_i}(\underset{\sim}{D}^{(i)})\}_{i=0}^{\infty}$, is monotonically increasing. Since this sequence is bounded by 100 as can be seen from (2.15), it must coverge to 100 (see, for example, Rudin 1976, p. 55), that is,

$$\lim_{i\to\infty} \Phi_{n_i}(\underset{\sim}{D}^{(i)}) = 100.$$

In Khuri (1985) it is further shown that (3.1) is in fact a strict inequality.

The addition of new runs to increase the percent rotatability is tantamount to "repairing" rotatability. Hebble and Mitchell (1972) have indirectly done so by maximizing the determinant $|\underset{\sim}{X}'\underset{\sim}{X}|$ through design augmentation, where $\underset{\sim}{X}$ is the matrix given in (1.1). The reason rotatability can be partially restored by their method is based on theoretical results by Wynn (1970) and Kiefer (1961). More specifically, the method of Hebble and Mitchell leads in the limit to a D-optimal design as was shown by Wynn (1970). On the other hand, Kiefer (1961) showed that D-optimal designs over a spherical region are rotatable.

4. EXAMPLES

Four numerical examples, 4.1 - 4.4, are presented in this

section in order to illustrate the applications of the measure of rotatability. The purpose of example 4.1 is to demonstrate the actual implementation of formula (2.15). Example 4.2 shows how the measure can be used to compare designs on the basis of their degrees of rotatability. Examples 4.3 and 4.4 serve to highlight the utility of the measure in repairing rotatability with the latter example describing an actual experimental situation.

Example 4.1

Consider fitting a second-order model of the form

$$E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 \qquad (4.1)$$

using a 3^2 factorial design with the j^{th} factor having the levels $-1,0,1(j=1,2)$. The coding described in (2.2) is already satisfied with $(j^2) = 6(j=1,2)$. In this case a=6, d=2, k=2, and n=9. The elements of the vectors $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$, $\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z})$, $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$, $\underset{\sim}{\omega}_0$, $\underset{\sim}{\omega}_2$, $\underset{\sim}{\omega}_4$, and the diagonal elements of the diagonal matrix $\underset{\sim}{A}$ (see 2.6 and 2.12) are given in Table 1. The value of $\min[Q_n(\underset{\sim}{D})]$ in (2.14) is .00555 and $\Phi_n(\underset{\sim}{D})$ in formula (2.15) is thus equal to 93.08. We conclude that the 3^2 factorial design is 93.08% rotatable.

Example 4.2: Roquemore's (1976) Hybrid Designs

These designs were introduced by Roquemore (1976) to emulate

certain characteristics of central composite or regular polyhedral designs. They are economical and are supposed to be near rotatable. Roquemore constructed three 3-variable designs, labeled by him as 310, 311A, and 311B, for a second-order model. These designs are reproduced in Table 2. He pointed out that the 311A design was the most nearly rotatable. This was based on observing contour plots of prediction variance and on a comparison of the values of the ratio $(j^4)/(j^2\ell^2)$, $j \neq \ell$, with the value 3 (this ratio must be equal to 3 in order for a design for a second-order model to be rotatable as can be verified from 1.4). By applying the measure of rotatability given in (2.15) it was found out that the percent rotatability values for the 310, 311A, and 311B designs were, respectively, 94.89, 99.40, and 98.99. This confirms Roquemore's assertion concerning the 311A design. It can also be seen that all three designs have high percent rotatability and that the 311B design is as nearly rotatable as the 311A design. Design 311B was also reported as the most efficient of the three designs with respect to both the D- and G-optimality criteria.

This example clearly shows that in conjuction with other measures of design efficiency, the rotatability measure can be utilized to select a design that possesses several characteristics of interest to the experimenter.

Example 4.3: Hebble and Mitchell (1972, Example 1, p. 769)

A second-order model in two input variables is fitted using the ten-point design $\underset{\sim}{D}^{(0)}$ described in Table 3. This design was originally planned as a rotatable central composite design with two center points. The region of interest, R, is circular with center at (0,0) and radius = 2. In terms of the coded variables, z_1 and z_2, the model is written as

$$E(y) = \gamma_0 + \gamma_1 z_1 + \gamma_2 z_2 + \gamma_{12} z_1 z_2 + \gamma_{11} z_1^2 + \gamma_{22} z_2^2 .$$

The percent rotatability of $\underset{\sim}{D}^{(0)}$ according to formula (2.15) is 80.65. This design was subsequently augmented with three additional repair points, one at a time, to get the sequence of designs, $\underset{\sim}{D}^{(1)}$, $\underset{\sim}{D}^{(2)}$, and $\underset{\sim}{D}^{(3)}$. As was described in Section 3, the design $\underset{\sim}{D}^{(i)}$ is obtained from the design $\underset{\sim}{D}^{(i-1)}$ by the addition of the point $\underset{\sim}{x}_i$ that maximizes $\Phi_{n_i}\left(\underset{\sim}{D}_{\underset{\sim}{x}}^{(i-1)}\right)$ with respect to $\underset{\sim}{x}$ over the region R(i=1,2,3). The maximization of Φ was carried out by using SEARCH, a computer program written by Conlon (1979) and is based on the controlled random search procedure introduced by Price (1977). The optimal locations of the additional three points and the corresponding percent rotatability of the ensuing designs, $\underset{\sim}{D}^{(1)}$, $\underset{\sim}{D}^{(2)}$, and $\underset{\sim}{D}^{(3)}$, are given in Table 4. Note that the first two points cause a sizable increase in the percent rotatability beyond the value 80.65 for the intitial design $\underset{\sim}{D}^{(0)}$. A total of

less than six seconds of CPU time was needed to locate the additional three points.

For each of the four designs, $\underset{\sim}{D}^{(0)}$, $\underset{\sim}{D}^{(1)}$, $\underset{\sim}{D}^{(2)}$, and $\underset{\sim}{D}^{(3)}$, contour plots of $\text{var}[\hat{y}(\underset{\sim}{z})]/\sigma^2$ were drawn within a region in the space of the coded variables which corresponds to R, where σ^2 is the random error variance and $\underset{\sim}{z} = (z_1, z_2)'$. These plots are shown in Figure 1. It can be clearly seen that the addition of the optimal three runs has caused the variance contours to have a much more circular appearance, particularly in the the case of run 13. This demonstrates the usefulness of the proposed measure as an effective tool to rectify nonrotatability.

Example 4.4

A company manufactures a liquid material for coating automobile window glass which when dried provides a barrier to ultraviolet rays and also reduces glare from the sun. The coating liquid consists of water combined with three active solid ingredients: a polymer (P), a coupling agent (CA), and a lubricant (L). A film is formed by passing the liquid through an extruder, oven drying it and then placing it on a roller.

An experiment is to be conducted consisting of several different combinations of the amounts of P, CA, and L with a fixed amount of water. The objective of the experiment is to determine the combination of P, CA, and L that is most effective in terms of

reducing light penetration. Light penetration is measured by taking a bright colored cloth affixed to the coated glass and exposing it to light for a fixed period of time. The color of the cloth is then compared to that of an unexposed piece of cloth of the same color and recording the degree of fading that has occurred. A low percent fade value is considered to be desirable.

In making up the combinations of water, polymer (P), coupling agent (CA), and lubricant (L) to produce the different coatings, a central composite rotatable design in P, CA, and L is set up. Listed in Table 5 are the amounts (in grams) of P, CA, and L to be combined with 2500 ml of water. The following transformation was applied so that the desing settings in the factorial portion have the familiar ±1 values:

$$x_1 = \frac{P-250}{25}, \quad x_2 = \frac{CA-22.5}{2.5}, \quad x_3 = \frac{L-7.5}{2.5}. \tag{4.2}$$

The design settings in terms of values of x_1, x_2, and x_3 are displayed in Table 6.

In this experiment, high ratios of the total amount of the active solid ingredients to water are considered undesirable because of problems with solubility. For the amount of water used (2500 ml), it was determined that a total of more than 305 gm of solid ingredients would be undesirable. From Table 5 we note that design points No. 8 and 10 fall in that category. Their settings had to be reduced to conform to the 305 upper bound constraint.

The experimenter chose to reduce the levels of P for these points from 275 and 292.05 to 262 and 275, respectively. The levels of CA and L were not altered. The total amounts of active solid ingredients for these two points are now 297 and 305 gm respectively. The design settings in terms of values of x_1, x_2, and x_3 for the resulting design are given in Table 6. The corresponding percent rotatability value is 81.69, a drop of 18.31% from the original central composite design. This clearly demonstrates the impact that this change of design settings has had on rotatability.

To recover the loss of rotatability, repair points were added to the central composite design with points No. 8 and 10 modified as was described earlier. The experimental region in the space of the x_1, x_2, and x_3 variables is a sphere of radius $\sqrt{3}$ centered at the origin. The first optimal point selected by the computer program SEARCH is shown in Table 6 as point No. 17. The corresponding total of P, CA, and L is 256.77 gm, which does not exceed the 305 limit. This point is therefore considered admissible. The percent rotatability value for the resulting 17-point design is 88.79. This represents a relative percent increase in rotatability of about 8.7. The second point selected by SEARCH increased the rotatability value to 95.31%. However, at this point $x_1 = 1.617$, $x_2 = .120$, and $x_3 = .119$, which results in a total of 321.023 gm of solid ingredients. The point is

inadmissible and was subsequently dropped. For the next point, the optimization was restricted to a smaller region, namely, a sphere of radius $\sqrt{.98}$ centered at the origin. The optimal point (No. 18 in Table 6) selected by SEARCH in this region was admissible with a corresponding total of 304.9 gm of solid ingredients. With the addition of the latter point, the rotatability value increased to 90.83%. At this stage, the sequential procedure was terminated. It was felt that additional points inside the smaller region would only produce marginal increases in the percent rotatability. To rapidly restore rotatability, SEARCH should be allowed to operate near the periphery of the experimental region (with radius equal to $\sqrt{3}$). In this example, however, this can lead to inadmissible points as was seen earlier.

5. CONCLUDING REMARKS

When a design is nonrotatable, it may be of interest to assess the extent of its departure from rotatability. This can be particularly useful in situations where a design is required to possess several desirable characteristics, including rotatability. It is important here not to confuse priorities when considering a choice of a response surface design. The introduction of the rotatability measure does not mean that rotatability should be emphasized at the expense of other design criteria. On the contrary, the variance and bias design criteria, for example, can

be by far more important. Only after these criteria (or perhaps others that may be of interest to the experimenter) have been fully pursued might one consider rotatability. In fact, rotatability may sometimes be compromised in favor of other desirable design features.

The measure of rotatability introduced in this paper gives the experimenter greater freedom and flexibility in selecting from a pool of efficient designs those that have high percent rotatability. These designs can be made even more rotatable, if necessary, by proper addition of design points as was shown in Section 3. Certainly, this action will not reduce the efficiency of the augmented designs.

ACKNOWLEDGEMENTS

I would like to thank the referees for their helpful comments and suggestions, which led to substantial improvements in the presentation of the material. I also wish to thank John A. Cornell for providing the data for Example 4.4. This research was partially supported by the Office of Naval Research Grant N00014-86-K-0059.

APPENDIX A: THE DERIVATION OF FORMULA (2.14)

The $\underset{\sim}{\omega}_{2m}$ vectors that appear in formula (2.9) are pairwise orthogonal. Formula (2.13) can therefore be written as

$$Q_n(\underset{\sim}{D}) = [\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z}) - \sum_{m=2}^{d} \kappa_{2m}\,\underset{\sim}{\omega}'_{2m}][\underset{\sim}{u}^{*}(\underset{\sim}{Z}'\underset{\sim}{Z}) - \sum_{m=2}^{d} \kappa_{2m}\,\underset{\sim}{\omega}_{2m}]$$

$$= \|\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2 - 2\sum_{m=2}^{d} \kappa_{2m}\,\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m}$$

$$+ \sum_{m=2}^{d} \kappa_{2m}^2\,\|\underset{\sim}{\omega}_{2m}\|^2. \tag{A.1}$$

By differentiating $Q_n(\underset{\sim}{D})$ with respect to $\kappa_{2m}(m=2,\ldots,d)$ and equating the derivatives to zero we get

$$\frac{\partial Q_n(\underset{\sim}{D})}{\partial \kappa_{2m}} = -2\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m} + 2\kappa_{2m}\|\underset{\sim}{\omega}_{2m}\|^2 = 0, \quad m=2,3,\ldots,d. \tag{A.2}$$

By solving for κ_{2m} we obtain

$$\kappa_{2m} = \underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\,\underset{\sim}{\omega}_{2m}/\|\,\underset{\sim}{\omega}_{2m}\|^2, \quad m=2,3,\ldots,d. \tag{A.3}$$

The solution (A.3) satisfies the constraint $\kappa_{2m} > 0$ $(m=2,3,\ldots,d)$ since $\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m} > 0$ for $m=2,3,\ldots,d$. This follows because $\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m}$ is a positive linear combination of the even design moments of order $\delta = 2m$ $(m=2,3,\ldots,d)$ for the design $\underset{\sim}{D}$. It is easy to verify that the solution (A.3) represents an absolute minimum that has the value

$$\min[Q_n(\underset{\sim}{D})] = \|\underset{\sim}{u}^{*}(\underset{\sim}{Z}'\underset{\sim}{Z})\|^2 - \sum_{m=2}^{d}[\underset{\sim}{u}^{*\prime}(\underset{\sim}{Z}'\underset{\sim}{Z})\underset{\sim}{\omega}_{2m}]^2/\|\underset{\sim}{\omega}_{2m}\|^2. \tag{A.4}$$

APPENDIX B: PROOF OF INEQUALITY (3.1)

Let $x_{uj}^{(i)}$ denote the u^{th} level of the j^{th} input variable for the design $\underset{\sim}{D}^{(i)}$ $(i=0,1,\ldots;\ j=1,2,\ldots,k;\ u=1,2,\ldots,n_i)$. Let $\bar{x}_j^{(i)} = \sum_{u=1}^{n_i} x_{uj}^{(i)}/n_i$ $(j=1,2,\ldots,k)$. The center of this design is the point $\underset{\sim}{\bar{x}}^{(i)} = (\bar{x}_1^{(i)}, \bar{x}_2^{(i)}, \ldots, \bar{x}_k^{(i)})'$. By condition (iii) in Section 2, the addition of this point to $\underset{\sim}{D}^{(i)}$ will not alter its measure of rotatability, that is,

$$\Phi_{n_{i+1}}\left(\underset{\sim}{D}^{(i)}_{\underset{\sim}{\bar{x}}^{(i)}}\right) = \Phi_{n_i}\left(\underset{\sim}{D}^{(i)}\right), \qquad i=0,1,\ldots\ . \tag{B.1}$$

Now, since

$$\Phi_{n_{i+1}}\left(\underset{\sim}{D}^{(i+1)}\right) = \max_{\underset{\sim}{x} \varepsilon R}\left[\Phi_{n_{i+1}}\left(\underset{\sim}{D}^{(i)}_{\underset{\sim}{x}}\right)\right], \quad i=0,1,\ldots\ , \tag{B.2}$$

then from (B.1) and (B.2) we obtain

$$\Phi_{n_i}\left(\underset{\sim}{D}^{(i)}\right) \le \Phi_{n_{i+1}}\left(\underset{\sim}{D}^{(i+1)}\right), \qquad i=0,1,\ldots\ . \tag{B.3}$$

Table 1. The Elements of the Vectors $\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$, $\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z})$, $\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$, $\underset{\sim}{\omega}_0$, $\underset{\sim}{\omega}_2$, $\underset{\sim}{\omega}_4$, and the Diagonal Elements of the Matrix $\underset{\sim}{A}$ for the 3^2 Factorial Design (Example 4.1)

$\underset{\sim}{v}(\underset{\sim}{Z}'\underset{\sim}{Z})$	$\underset{\sim}{A}$	$\underset{\sim}{u}(\underset{\sim}{Z}'\underset{\sim}{Z})$	$\underset{\sim}{u}^*(\underset{\sim}{Z}'\underset{\sim}{Z})$	$\underset{\sim}{\omega}_0$	$\underset{\sim}{\omega}_2$	$\underset{\sim}{\omega}_4$
9	1	9	0	1	0	0
0	$6^{-1/2}$	0	0	0	0	0
0	$6^{-1/2}$	0	0	0	0	0
0	6^{-1}	0	0	0	0	0
6	6^{-1}	1	0	0	1	0
6	6^{-1}	1	0	0	1	0
6	6^{-1}	1	0	0	1	0
0	6^{-1}	0	0	0	0	0
0	$6^{-3/2}$	0	0	0	0	0
0	$6^{-3/2}$	0	0	0	0	0
0	$6^{-3/2}$	0	0	0	0	0
6	6^{-1}	1	0	0	1	0
0	$6^{-3/2}$	0	0	0	0	0
0	$6^{-3/2}$	0	0	0	0	0
0	$6^{-3/2}$	0	0	0	0	0
4	6^{-2}	4/36	4/36	0	0	1
0	6^{-2}	0	0	0	0	0
0	6^{-2}	0	0	0	0	0
6	6^{-2}	6/36	6/36	0	0	3
4	6^{-2}	4/36	4/36	0	0	1
6	6^{-2}	6/36	6/36	0	0	3

Table 2. Roquemore's (1976) Three-Variable Hybrid Designs (Example 4.2)*

310			311A			311B		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0	0	1.2906	0	0	2	0	0	$6^{1/2}$
0	0	-.136	0	0	-2	0	0	$-6^{1/2}$
-1	-1	.6386	$-2^{1/2}$	$-2^{1/2}$	1	-.7507	2.1063	1
1	-1	.6386	$2^{1/2}$	$-2^{1/2}$	1	2.1063	.7507	1
-1	1	.6386	$-2^{1/2}$	$2^{1/2}$	1	.7507	-2.1063	1
1	1	.6386	$2^{1/2}$	$2^{1/2}$	1	-2.1063	-.7507	1
1.1736	0	-.9273	2	0	-1	.7507	2.1063	-1
-1.1736	0	-.9273	-2	0	-1	2.1063	-.7507	-1
0	1.1736	-.9273	0	2	-1	-.7507	-2.1063	-1
0	-1.1736	-.9273	0	-2	-1	-2.1063	.7507	-1
			0	0	0	0	0	0

* The first digit in a design title is the number of variables, the next two digits are the number of points. A letter differentiates designs of the same size.

Table 3. The Initial Nonrotatable Design $\underset{\sim}{D}^{(0)}$ (Example 4.3)

x_1	x_2
-1	1.35
1	-1.25
-1.6	- .85
1	1
-1.5	0
1.55	0
0	-1
0	1.55
.55	.30
0	0

Table 4. Repair Points and Percent Rotatability Values for the Corresponding Augmented Designs for Example 4.3 (The Initial Design is Given in Table 3 and has a Percent Rotatability Value of 80.65)

Run No.	x_1	x_2	Augmented Design	% Rotatability	Increase in % Rotatability
11	-.1188	-1.8593	$\underset{\sim}{D}^{(1)} = \underset{\sim}{D}^{(0)}$ Plus Run No. 11	89.99	9.34
12	-.8295	.0091	$\underset{\sim}{D}^{(2)} = \underset{\sim}{D}^{(1)}$ Plus Run No. 12	96.47	15.82
13	-.1450	-.2764	$\underset{\sim}{D}^{(3)} = \underset{\sim}{D}^{(2)}$ Plus Run No. 13	97.03	16.38

Table 5. The Actual Levels (in grams) of P, CA, and L to be Combined with 2500 ml of Water for the Central Composite Rotatable Design of Example 4.4

Run No.	P	CA	L	Total Amount of Active Solids
1	225.0	20.0	5.0	250.0
2	275.0	20.0	5.0	300.0
3	225.0	25.0	5.0	255.0
4	275.0	25.0	5.0	305.0
5	225.0	20.0	10.0	255.0
6	275.0	20.0	10.0	305.0
7	225.0	25.0	10.0	260.0
8	275.0	25.0	10.0	310.0*
9	207.95	22.5	7.5	237.95
10	292.05	22.5	7.5	322.05*
11	250.0	18.295	7.5	275.795
12	250.0	26.705	7.5	284.205
13	250.0	22.5	3.295	275.795
14	250.0	22.5	11.705	284.205
15	250.0	22.5	7.5	280.0
16	250.0	22.5	7.5	280.0

*The total exceeds 305 gm.

TABLE 6. The Rotatable Central Composite Design Under the Coding of Eqs. (4.2), the Design Settings for the Modified Design with the Additional Repair Points, and the Corresponding Rotatability Values (Example 4.4)

Run No.	Rotatable Central Composite Design			Modified Central Composite Design			% Rotatability
	x_1	x_2	x_3	x_1	x_2	x_3	
1	-1	-1	-1	-1	-1	-1	
2	1	-1	-1	1	-1	-1	
3	-1	1	-1	-1	1	-1	
4	1	1	-1	1	1	-1	
5	-1	-1	1	-1	-1	1	
6	1	-1	1	1	-1	1	
7	-1	1	1	-1	1	1	
8	1	1	1	.48	1	1	
9	-1.682	0	0	-1.682	0	0	
10	1.682	0	0	1	0	0	
11	0	-1.682	0	0	-1.682	0	
12	0	1.682	0	0	1.682	0	
13	0	0	-1.682	0	0	-1.682	
14	0	0	1.682	0	0	1.682	
15	0	0	0	0	0	0	
16	0	0	0	0	0	0	81.69
17*				-.828	-.506	-.506	88.79
18*				.966	.151	.151	90.83

*Repair points

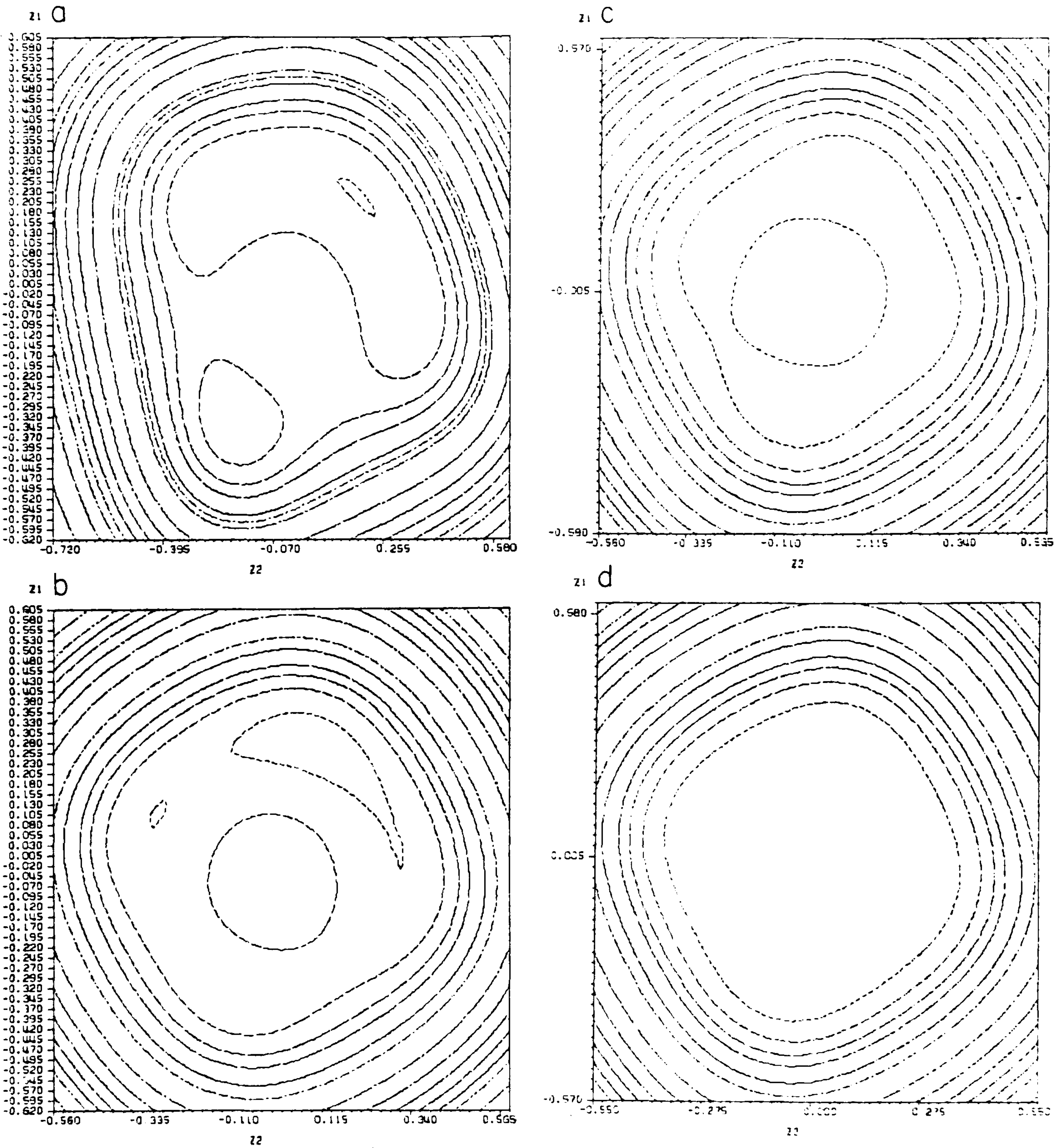


Figure 1. Contour Plots of $\mathrm{var}[\hat{y}(\underset{\sim}{z})]/\sigma^2$ For

(a) $\underset{\sim}{D}^{(0)}$, the initial ten-point design given in Table 3.

(b) $\underset{\sim}{D}^{(1)}$, the design $\underset{\sim}{D}^{(0)}$ augmented with (-.1188, -1.8593).

(c) $\underset{\sim}{D}^{(2)}$, the design $\underset{\sim}{D}^{(1)}$ augmented with (-.8295, .0091).

(d) $\underset{\sim}{D}^{(3)}$, the design $\underset{\sim}{D}^{(2)}$ augmented with (-.1450, -.2764).

REFERENCES

Box, G.E.P., and Hunter, J.S. (1957), "Multi-Factor Experimental Designs for Exploring Response Surfaces," Annals of Mathematical Statistics, 28, 195-241.

Conlon, M. (1979), "SEARCH: A Controlled Random Search Procedure for Function Minimization," a handout issued by the Center for Instructional and Research Computing Activities, 411 Weil Hall, University of Florida, Gainesville, FL 32611.

Hebble, T.L., and Mitchell, T.J. (1972), "Repairing Response Surface Designs," Technometrics, 14, 767-779.

Khuri, A.I., and Myers, R.H. (1979), "Modified Ridge Analysis", Technometrics, 21, 467-473.

Khuri, A.I. (1985), "A Measure of Rotatability for Response Surface Designs", Technical Report Number 232, Department of Statistics, University of Florida, Gainesville, FL 32611.

Kiefer, J. (1961), "Optimum Experimental Designs V, With Applications to Systematic and Rotatable Designs," Proceedings of the Fourth Berkeley Symposium, Vol. I, University of California Press, 381-405.

Littell, R.C., and Mott, G.O. (1974), "Computer Assisted Design and Analysis of Response Surface Experiments in Agronomy," Soil and Crop Science Society of Florida Proceedings, 34, 94-97.

Myers, R.H. (1976), Response Surface Methodology, Ann Arbor, MI: Edwards Brothers (distributors).

Price, W.L. (1977), "A Controlled Random Search Procedure for Global Optimization," Computer Journal, 20, 367-370.

Roquemore, K.G. (1976), "Hybrid Designs for Quadratic Response Surfaces," Technometrics, 18, 419-423.

Rudin, W. (1976), Principles of Mathematical Analysis (3rd ed.), New York: McGraw-Hill.

Wynn, H.P. (1970), "The Sequential Generation of D-Optimum Experimental Designs," Annals of Mathematical Statistics, 41, 1655-1664.

END
6-81
DTIC